

Niridazole
61-57-4 | DTXSID6045244

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 341 °C

Global applicability domain: Outside

Local applicability domain index: 1.76e-01

Confidence level: 6.92e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>3-Methyl-1-phenyl-1H-pyrazol-5-amine</div> <div>Measured: 333</div> <div>Predicted: 334</div>	<div>Image not found</div> <div>2,4-Dinitroaniline</div> <div>Measured: 334</div> <div>Predicted: 330</div>	<div>Image not found</div> <div>4-Aminoazobenzene</div> <div>Measured: 366</div> <div>Predicted: 337</div>
<div>Image not found</div> <div>Pendimethalin</div> <div>Measured: 330</div> <div>Predicted: 335</div>	<div>Image not found</div> <div>Desmetryn</div> <div>Measured: 345</div> <div>Predicted: 341</div>	